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Comparative Study of Fullerene Derivatives in High Performance PNTz4T based OPV

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Introduction

Since 2009, the power conversion efficiency (PCE) of organic photovoltaic (OPV) cells has been rapidly increasing. This sudden increase in device performances is mostly related to the synthesis of novel materials. More specifically, the introduction of p-type polymers with alternating electron-rich and electron-poor building units combined with newly developed fullerene derivatives result in PCE approaching 10%.[1] In this study, we focus on a polymer based on quaterthiophene and naphthobisthiadiazole units (PNTz4T).[2]

Results and Discussion

Three fullerene derivatives, namely, $PC_{61}BM$, $PC_{71}BM$ and ICBA, were selected as potential electron acceptors in regular device architectures (Figure 1). The resulting average PCE are 7.52, 8.52 and 2.58% for $PC_{61}BM$, $PC_{71}BM$ and ICBA, respectively.

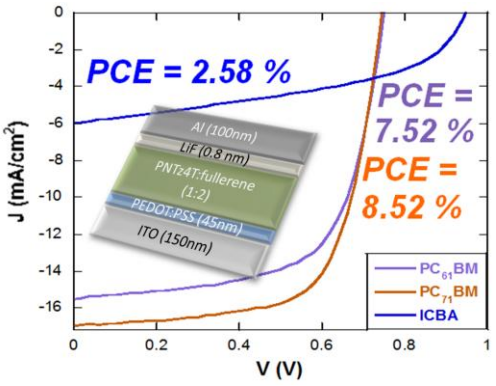

Figure 1: Device architecture and J-V characteristics of PNTz4T based OPV cells

The two PCBM acceptors exhibit very high Jsc which originates from the wide absorption of the donor and high crystallinity of both donor and acceptor molecules. Higher Jsc can be observed with $PC_{71}BM$ which is partially related to its higher contribution to sunlight absorption. PNTz4T:ICBA devices, on the other hand, exhibit a high Voc (almost 1V), but lower values of Jsc and FF.

Through a careful and systematic study, we investigated the origins of the differences observed in devices performances. In fact, XRD measurements reveal that, unlike PCBM, ICBA shows very low crystallinity. As fullerene crystallinity is closely related to the electron transporting properties of the acceptor molecule in the devices, we prepared hole- and electron-only devices to study the charge balance through the various active layers. We demonstrate that the performances (especially FF) can be correlated to the charge balance in the various device types which explains not only the high PCE observed in PCBM devices but also the lower Jsc and FF in ICBA devices.

We therefore demonstrated that fabricating high performances polymer solar cells not only requires carefully designing and selecting the active materials in order to obtain the ideal morphology and optical properties but that a particular attention should also be given to charge balance to reach high FF and PCE.

References

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